

WHAT IS CLAIMED IS:

1. A method of forming a combinatorial library of compounds, the method comprising reacting a plurality of core molecules with a mixture of nucleophilic building blocks in a reaction vessel to form a library of compounds, wherein each of  
5 said core molecules comprises (i) an acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional group; and (ii) an aldehyde or ketone functional group.

2. The method of claim 1, wherein the mixture of nucleophilic building blocks comprises at least one amine.

10 3. The method of claim 1, wherein substantially all of the nucleophilic building blocks are amines.

4. The method of claim 1, wherein substantially all of the core molecules are the same.

15 5. The method of claim 1, wherein the plurality of core molecules comprises at least two different core molecules.

20 6. The method of claim 3, wherein the set of nucleophilic building blocks that are each contacted with and can each react with the acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester reactive centers are different from the set of nucleophilic building blocks that are each contacted with and can each react with the aldehyde or ketone reactive centers.

7. The method of claim 4, wherein the core molecule comprises two acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional groups.

8. The method of claim 4, wherein the core molecule comprises three acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional groups.

9. The method of claim 1, wherein each of said core molecules comprises an  
5 activated ester group.

10. The method of claim 9, wherein the activated ester group is a pentafluorophenyl ester group.

11. The method of claim 9, wherein the activated ester group is a dinitrophenyl ester group.

12. The method of claim 1, wherein the aldehyde or ketone functional group  
10 is a terminal aldehyde or ketone.

13. The method of claim 1, wherein said core molecule has the formula A-B-C,  
wherein

15 B comprises from 1 to about 4 carbocyclic or heterocyclic rings, any of which rings may be optionally substituted, and wherein A and C may be attached to the same or different rings;

A is an organic moiety comprising an acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional group;  
and

20 C is an organic moiety comprising an aldehyde or ketone functional group.

14. The method of claim 13, wherein at least one of the rings is an aromatic ring.

15. The method of claim 13, wherein B comprises a fused bicyclic or tricyclic ring system.

16. The method of claim 13, wherein B comprises two rings connected by a covalent bond.

5 17. The method of claim 13, wherein A and C are attached to the same ring.

18. The method of claim 14, wherein the ring to which A and C are attached is a benzene ring.

19. The method of claim 13, wherein

A has the formula  $-Y^1-W$ , where:

10 W is an isocyanate or isocyanate equivalent, acid halide, or sulfonyl halide functional group, or W has the formula  $-C(O)-OR^1$ , where  $R^1$  is selected from the group consisting of haloalkyl and aryl substituted with at least one electron withdrawing substituent, or  $-OR^1$  is a radical formed by deprotonation of an *N*-hydroxyheterocycle or *N*-hydroxyimide;

15  $Y^1$  is absent or comprises a linking chain of from 1 to about 6 contiguous atoms independently selected from the group consisting of carbon, nitrogen, oxygen, or sulfur, wherein the carbon and nitrogen atoms may be optionally substituted and the nitrogen and sulfur atoms may be optionally oxidized, and wherein any of the contiguous atoms of the  
20 chemical linkage may form part of a ring structure; and

C has the formula  $-Y^2-Z$ , where  $Y^2$  is as defined above for  $Y^1$  and Z is an aldehyde or ketone.

20. The method of claim 19, wherein  $R^1$  is selected from the group consisting of succinimide, phthalimide, perfluoroalkyl, pentafluorophenyl, dinitrophenyl,

nitrophenyl, difluorophenyl, fluorophenyl, trifluorophenyl, chlorophenyl,  
dichlorophenyl, chloronitrophenyl, and tetrafluoronitrophenyl.

21. The method of claim 19, wherein W is selected from the group consisting  
of acid halide, sulfonyl halide, dinitrophenyl ester, and pentafluorophenyl ester.

5 22. The method of claim 19, wherein Y<sup>1</sup> comprises a W group.

23. The method of claim 19, wherein Y<sup>2</sup> comprises a W group.

24. The method of claim 19, wherein the Y<sup>1</sup> or Y<sup>2</sup> linking chain comprises an  
ester, amide or sulfonamide linkage.

10 25. The method of claim 19, wherein the Y<sup>1</sup> or Y<sup>2</sup> linking chain comprises an  
ether linkage.

26. The method of claim 19, wherein the Y<sup>2</sup> linking chain comprises a ring and  
the aldehyde or ketone functional group is attached to the ring.

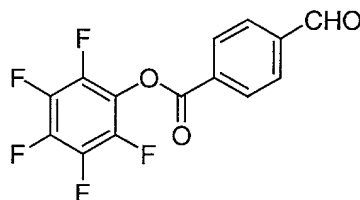
27. The method of claim 1, wherein said mixture of amines comprises primary  
amines.

15 28. The method of claim 1, wherein at least 90% of said library compounds  
each comprise a secondary amine functional group and an amide, sulfonamide, urea,  
ester, carbamate, or sulfonate ester functional group.

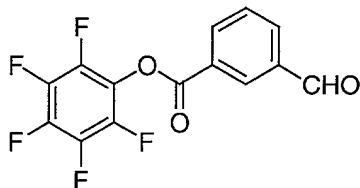
20 29. The method of claim 28, wherein at least 95% of said library compounds  
each comprise a secondary amine functional group and an amide, sulfonamide, urea,  
ester, carbamate, or sulfonate ester functional group.

30. The method of claim 29, wherein at least 99% of said library compounds each comprise a secondary amine functional group and an amide, sulfonamide, urea, ester, carbamate, or sulfonate ester functional group.

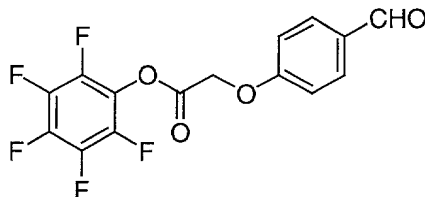
31. A method of forming a combinatorial library of compounds, the method  
5 comprising reacting a plurality of core molecules with a mixture of nucleophilic building blocks in a reaction vessel to form a library of compounds, wherein substantially all of the core molecules have the formula



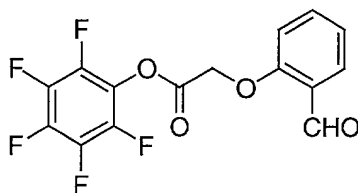
32. A method of forming a combinatorial library of compounds, the method  
10 comprising reacting a plurality of core molecules with a mixture of nucleophilic building blocks in a reaction vessel to form a library of compounds, wherein substantially all of the core molecules have the formula



33. A method of forming a combinatorial library of compounds, the method  
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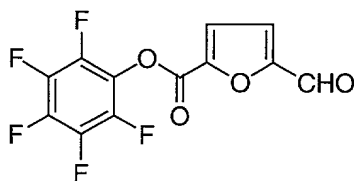


34. A method of forming a combinatorial library of compounds, the method comprising reacting a plurality of core molecules with a mixture of nucleophilic building blocks in a reaction vessel to form a library of compounds, wherein substantially all of the core molecules have the formula



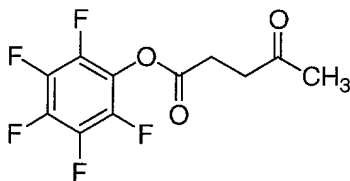
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35. A method of forming a combinatorial library of compounds, the method comprising reacting a plurality of core molecules with a mixture of nucleophilic building blocks in a reaction vessel to form a library of compounds, wherein substantially all of the core molecules have the formula



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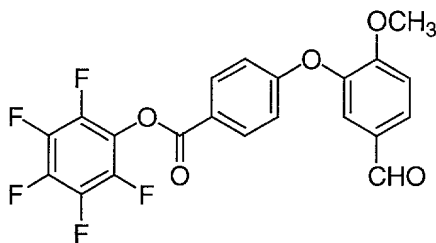
36. A method of forming a combinatorial library of compounds, the method comprising reacting a plurality of core molecules with a mixture of nucleophilic building blocks in a reaction vessel to form a library of compounds, wherein substantially all of the core molecules have the formula



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37. A method of forming a combinatorial library of compounds, the method comprising reacting a plurality of core molecules with a mixture of nucleophilic

building blocks in a reaction vessel to form a library of compounds, wherein substantially all of the core molecules have the formula



38. A combinatorial library of compounds, wherein said compounds are produced by reacting a plurality of core molecules with a mixture of nucleophilic building blocks, wherein the core molecule comprises (i) an acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional group; and (ii) an aldehyde or ketone functional group.

39. The library of claim 38, wherein said reacting step comprises sequentially (i) contacting the core molecules with a mixture of building blocks so that reaction with the acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional groups is achieved and reaction with aldehyde or ketone functional groups is also achieved to form a mixture of intermediate compounds comprising imine groups; and

(ii) adding a reducing agent to reduce the imine groups formed in step (i).

40. The library of claim 38, wherein said reacting step comprises sequentially (i) contacting the core molecules with a mixture of amine building blocks so that reaction with the acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional groups is achieved to produce a first mixture of intermediate compounds;

(ii) contacting the first mixture of intermediate compounds with a mixture of amine building blocks so that reaction with the aldehyde or ketone functional groups is achieved to form a second mixture of intermediate compounds comprising imine groups; and

5 (ii) contacting the second mixture of intermediate compounds with a reducing agent to reduce the imine groups formed in step (i).

41. A compound having the formula A-B-C, wherein

B comprises from 1 to about 4 carbocyclic or heterocyclic rings, any of which rings may be optionally substituted, and wherein A and C may be attached to the same or different rings;

A is an organic moiety comprising an acid halide, sulfonyl halide, isocyanate or isocyanate equivalent, or activated ester functional group; and

C is an organic moiety comprising an aldehyde or ketone functional group.